CHARACTERIZATION OF INTERMOLECULAR INTERACTIONS AT PLAY IN THE 2,2,2-TRIFLUOROETHANOL TRIMERS USING CAVITY AND CHIRPED-PULSE MICROWAVE SPECTROSCOPY

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2,2,2-trifluoroethanol (TFE) is a common aqueous co-solvent in biological chemistry which may induce or destabilize secondary structures of proteins and polypeptides, thanks to its diverse intermolecular linkages originating from the hydrogen bonding potential of both the hydroxyl and perfluoro groups.[a] Theoretically, the TFE monomer is predicted to have two stable *gauche* (*gauche*$^+$/*gauche*$^-$) conformations whereas the *trans* form is unstable or is supported only by a very shallow potential. Only the gauche conformers have been identified in the gas phase, whereas liquid phase studies suggest a *trans*:*gauche* ratio of 2:3.[b] The question at which sample (cluster) size the *trans* form of TFE would appear was one major motivation for our study.

Here, we report the detection of three trimers of TFE using Balle-Flygare cavity and chirped-pulse Fourier transform microwave spectroscopy (CP-FTMW) techniques. The most stable observed trimer features one *trans*- and two *gauche*-TFE subunits. The other two trimers, observed using a newly constructed 2-6 GHz CP-FTMW spectrometer, consist of only the two *gauche* conformers of TFE. Quantum Theory of Atoms in Molecules (QTAIM)[c] and non-covalent interactions (NCI)[d] analyses give detailed insights into which intermolecular interactions are at play to stabilize the *trans* form of TFE in the most stable trimer.

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[c] R. F. W. Bader, Chem. Rev. 1991, 91, 893-928.

[d] E. R. Johnson, S. Keinan, P. Mori-Sánchez, J. Contreras-Garcia, A. J. Cohen, W. Yang, J. Am. Chem. Soc., 2010, 132, 6498-6506.